# 1-tert-Butoxy-2-propanol, heptafluorobutyrate

**Inchi:** InChI=1S/C11H15F7O3/c1-6(5-20-8(2,3)4)21-7(19)9(12,13)10(14,15)11(16,17)18/h6H,5
**InchiKey:** TTXDLKZACJODPX-UHFFFAOYSA-N
**Formula:** C11H15F7O3
**SMILES:** CC(COC(C)(C)C)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 328.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1651.93 | kJ/mol | Joback Method |
| hf | -2060.44 | kJ/mol | Joback Method |
| hfus | 16.60 | kJ/mol | Joback Method |
| hvap | 40.36 | kJ/mol | Joback Method |
| log10ws | -3.89 | | Crippen Method |
| logp | 3.566 | | Crippen Method |
| mcvol | 191.550 | ml/mol | McGowan Method |
| pc | 1631.17 | kPa | Joback Method |
| rinpol | 959.00 | | NIST Webbook |
| rinpol | 959.00 | | NIST Webbook |
| tb | 531.32 | K | Joback Method |
| tc | 689.39 | K | Joback Method |
| tf | 306.93 | K | Joback Method |
| vc | 0.769 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 511.48 | J/mol×K | 531.32 | Joback Method |
| cpg | 525.63 | J/mol×K | 557.67 | Joback Method |
| cpg | 538.95 | J/mol×K | 584.01 | Joback Method |
| cpg | 551.49 | J/mol×K | 610.36 | Joback Method |
| cpg | 563.28 | J/mol×K | 636.70 | Joback Method |
| cpg | 574.36 | J/mol×K | 663.05 | Joback Method |
| cpg | 584.76 | J/mol×K | 689.39 | Joback Method |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U378347&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |